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ABSTRACT

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1. Introduction

Stochastic models of computer systems often result in Markov chains with a very large number of states. For example, a closed exponential queuing network with K servers and N customers may generate a chain that grows like $N^K/K!$ as N becomes large. In order to determine the steady-state probability vector of a very large chain it is necessary to exploit any special structure that the underlying system may have.

In this paper we shall be concerned with *nearly uncoupled* Markov chains (also known as nearly completely decomposable Markov chains). These chains model systems whose components can be clustered into loosely coupled aggregates of tightly interacting states. Mathematically, the states of such chains can be ordered so that the state transition probability matrix has the form

$$A = \begin{pmatrix} A_{11} & E_{12} & \cdots & E_{1l} \\ E_{21} & A_{22} & \cdots & E_{2l} \\ \vdots & \vdots & & \vdots \\ E_{l1} & E_{l2} & \cdots & A_{ll} \end{pmatrix} \tag{1.1}$$

where the off-diagonal blocks E_{ij} are small compared to the diagonal blocks A_{ii}. For later use we shall write

$$A = D + E, \tag{1.2}$$

where

$$D = \operatorname{diag}(A_{11}, A_{22}, \ldots, A_{ll}), \tag{1.3}$$

and set

$$\epsilon = \|E\|, \tag{1.4}$$

where $\|\cdot\|$ denotes the spectral norm [7, Ch. 4].

Since A is stochastic, it satisfies

$$Ax = x, \tag{1.5}$$

where x denotes the vector whose components are all one. We shall assume that the chain is irreducible and aperiodic [3, Ch. 2], so that there is a unique, positive steady state vector y that satisfies

$$y^{\mathrm{T}}A = y^{\mathrm{T}} \tag{1.6}$$

and

$$y^{\mathrm{T}}x = 1. \tag{1.7}$$

The purpose of this paper is to introduce a composite algorithm for computing y. The proposed algorithm is iterative, each iteration consisting of two parts — a sequence of *block Gauss–Seidel steps* followed by a *Rayleigh–Ritz refinement.* We shall now describe each step in detail.

The block Gauss–Seidel step is the iteration commonly used to solve the large linear systems arising in the numerical treatment of partial differential equations [11]. In this case we apply it to the system

$$y^{\mathrm{T}}(I - A) = 0, \tag{1.8}$$

which is equivalent to (1.6). Let z denote the current approximation to y, and partition z conformally with the partitioning of A in (1.1):

$$z^{\mathrm{T}} = (z_1^{\mathrm{T}}\ z_2^{\mathrm{T}}\ \ldots\ z_l^{\mathrm{T}}). \tag{1.9}$$

The block Gauss–Seidel iteration produces a new approximation $\tilde{z}$ to y according to the formula

$$\tilde{z}_j^{\mathrm{T}} = \Big(\sum_{i<j} \tilde{z}_i^{\mathrm{T}}E_{ij} + \sum_{i>j} z_i^{\mathrm{T}}E_{ij}\Big)(I - A_{jj})^{-1} \qquad (j = 1, 2, \ldots, l). \tag{1.10}$$

In other words $\tilde{z}_j$ is just the vector obtained by solving the jth row of the partitioned form of (1.8) while holding $\tilde{z}_1 \ldots \tilde{z}_{j-1}$ and $z_{j+1} \ldots z_l$ fixed.

The Rayleigh–Ritz step is a standard method for extracting an approximate eigenvector from a subspace that nearly contains the eigenvector. Again let z, the current approximation to y, be partitioned as in (1.9), and assume that the components of z are positive. Let $\hat{z}_j = z_j/\|z_j\|_1$, where $\|\cdot\|_1$ denotes the 1-norm [7, Ch. 4]. The space from which the new approximation $\tilde{z}$ is to be extracted is spanned by the columns of the matrix

$$T_z = \begin{pmatrix} \hat{z}_1 & 0 & \cdots & 0 \\ 0 & \hat{z}_2 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \hat{z}_l \end{pmatrix}. \tag{1.11}$$

The algorithm goes as follows. Set

$$S = \begin{pmatrix} x_1 & 0 & \cdots & 0 \\ 0 & x_2 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & x_l \end{pmatrix}, \tag{1.12}$$

where the x_i are from a partition of x conformal with (1.1). Compute

$$B_z = T_z^{\mathrm{T}} A S. \tag{1.13}$$

It is easily verified that B_z is an irreducible, aperiodic, stochastic matrix and therefore has a unique, positive eigenvector v_z that satisfies

$$v_z^{\mathrm{T}} B_z = v_z^{\mathrm{T}} \qquad (\|v_z\|_1 = 1). \tag{1.14}$$

The new approximation $\tilde{z}$ to y is given by

$$\tilde{z} = T_z v_z. \tag{1.15}$$

The iteration proposed here consists of alternating sequences of Gauss–Seidel and Rayleigh–Ritz steps. In the next two sections of this paper we shall give a mathematical analysis of this method. However, the treatment is quite involved, and it is appropriate to summarize our results here. Those who are uninterested in the supporting details should pass directly from the end of this section to §4, where implementation issues are discussed.

Provided certain regularity conditions are satisfied, our results hold for all sufficiently small ϵ. In Section 2 it will be shown that the vector z can be written in the form

$$z = y + Y_2 g_2 + Y_3 g_3, \tag{1.16}$$

where Y_2 is an $n \times (l-1)$ matrix and Y_3 is an $n \times (n-l)$ matrix, both constructed from the matrix A. If we set

$$\gamma_i = \|g_i\| \qquad (i = 2, 3), \tag{1.17}$$

then the sizes of the γ_i tell how good an approximation z is to y. It turns out that the Gauss–Seidel step reduces γ_3 by a factor of order ϵ. The subsequent Rayleigh–Ritz step reduces γ_2, again by a factor of order ϵ. Thus the composite iteration reduces the error by a factor of order ϵ. Both steps are necessary, since the Gauss–Seidel step may reduce γ_2 only slowly, while the Rayleigh–Ritz step is stationary after one application (because $T_z = T_{\hat{z}}$).

In this paper we shall analyze only the Gauss–Seidel step, since the Rayleigh–Ritz step has been analyzed elsewhere [4]. The latter is closely related to methods of aggregation, which were first proposed in this connection by Simon and Ando [5]. The idea is to determine a vector z such that T_z is a good approximation to T_y and then apply a Rayleigh–Ritz step to approximate y. The diagonals of T_z are usually found by solving eigenvalue problems associated with with the A_{ii}. For example, Stewart [8] takes the $\hat{z}_i$ to be the normalized left eigenvectors of the A_{ii}; Courtois [1] takes them to be the normalized left eigenvectors of stochastic approximations A_{ii}^* to the A_{ii}. Under appropriate assumptions, either method produces an $O(\epsilon)$ approximation to y.

The drawback of this form of aggregation is that it produces a single result, which may or may not be accurate enough. To remedy this defect, two workers have proposed composite iterative schemes that reduce the error by a factor of order ϵ. Takahashi [9] has proposed a method that turns out to be very close to the one analyzed here; so close, in fact, that the analysis of our method may be easily extended to prove the convergence of his.

The method of Vantilborgh [10] is quite different in character. He uses an approximation to y to construct stochastic matrices A_{ii}^*, each with the property that its steady-state vector $\hat{z}_i$ is an improved approximation to the corresponding part of y, suitably normalized. These vectors are used in a Rayleigh–Ritz step, as described above. Vantilborgh indicates that when this process is iterated, it provides an $O(\epsilon)$ reduction in the error for each step. The chief drawback of the

algorithm is that it requires the solution of l eigenvalue problems to compute the $\hat{z}_i$.

The paper is organized as follows. In the next section material from [4] on the structure of nearly uncoupled Markov chains is reviewed. Careful attention will be devoted to the conditions that must obtain as ϵ approaches zero in order for our results to be valid. In §3 the Gauss–Seidel step is analyzed. The paper concludes with a section containing a discussion of the computational issues and an example.

2. The Structure of Nearly Uncoupled Markov Chains

In this section we shall review some results found in [4] on the structure of nearly uncoupled Markov chains. The purpose is twofold. First, among the results is a precise statement of the behavior of the Rayleigh–Ritz refinement. Second, the notation and results are needed to establish the properties of the Gauss–Seidel step.

We wish for our results to hold uniformly as ϵ approaches zero; i.e., as A approaches a block diagonal matrix. This requires that we restrict the way in which A approaches block diagonality; for very simple counter examples show that a small ϵ is not by itself sufficient to guarantee the structure usually associated with nearly uncoupled matrices. One approach is to assume a specific parameterization for A. For example, in [1] and [10] it is assumed that A can be written in the form

$$A = A^* + \epsilon B, \tag{2.1}$$

where A^* is a block diagonal stochastic matrix. Although this approach works, it has two drawbacks. First, it does not allow the elements of E to approach zero other than linearly. Second, it presupposes that the approach to the limit is along the fixed path determined by the matrix B. We therefore prefer to place different restrictions on the behavior of A as ϵ approaches zero, restrictions which at once overcome the above drawbacks and give insight into how the theory can fail.

The first condition specifies how the components of y behave. Write

$$y^{\mathrm{T}} = (y_1^{\mathrm{T}}\ y_2^{\mathrm{T}}\ \ldots\ y_l^{\mathrm{T}}), \tag{2.2}$$

where the partitioning is conformal with the underlying partition of the chain. Then we require the following for our first condition.

Regularity Condition 1. There is a constant $m_1 > 0$ such that

$$\|y_i\|_1 \geq m_1 \qquad (i = 1, 2, \ldots, l). \tag{2.3}$$

This condition is related to the asymptotic block irreducibility of A. Specifically, set $\hat{y}_i = y_i / \|y_i\|_1$ and let B_y be defined in analogy with (1.13). Then the diagonal elements $\hat{y}_i^{\mathrm{T}} A_{ii} x_i$ of B_y approach one, while the off-diagonal elements $\hat{y}_i^{\mathrm{T}} E_{ij} x_j$ approach zero at least as fast as ϵ. If some of the off-diagonal elements of B_y were to approach zero faster than others in such a way that B_y approaches reducibility, then one would expect some of the components of the left eigenvector v_y of B_y to approach zero. But it is easily verified that

$$v_y^{\mathrm{T}} = (\|y_1\|_1, \|y_2\|_1, \ldots, \|y_l\|_1). \tag{2.4}$$

Thus (2.3) guards against the effects of asymptotic reducibility.

The second condition requires some further notation. In [4] it is shown that there are matrices J_i and K_i such that

$$(x_i \; J_i)^{-1} = (\hat{y}_i \; K_i)^{\mathrm{T}} \qquad (i = 1, 2, \ldots, l). \tag{2.5}$$

Moreover, for $i = 1, 2, \ldots, l$ the norms of the J_i and K_i are bounded by quantities that are independent of ϵ. Let

$$(\hat{y}_i \; K_i)^{\mathrm{T}} A_{ii} (x_i \; J_i) = \begin{pmatrix} \beta_i & h_i^{\mathrm{T}} \\ g_i & C_i \end{pmatrix} \qquad (i = 1, 2, \ldots, l). \tag{2.6}$$

Our second regularity condition may now be stated as follows.

Regularity Condition 2. There is a constant M_2 such that

$$\|(I - C_i)^{-1}\| < M_2 \qquad (i = 1, 2, \ldots, l). \tag{2.7}$$

This condition circumscribes the behavior of the smallest $n - l$ eigenvalues of A. To see this, note that as ϵ approaches zero, the eigenvalues of A approach those of the A_{ii}, or equivalently those of the matrices (2.6), which by (2.5) are similar to the A_{ii}. Now it is shown in [4] that g and h approach zero as ϵ approaches zero, and it is easy to verify that the β_i approach one. Thus the smallest $n - l$ eigenvalues of A approach the eigenvalues of the C_i. Since the norm of a matrix is a bound on its eigenvalues, if c denotes any eigenvalue of C_i then it follows from (2.7) that $|1 - c|^{-1} < M_2$, or equivalently

$$|1 - c| > \frac{1}{M_2}. \tag{2.8}$$

Thus the second regularity condition insures that the smallest $n-l$ eigenvalues of A remain uniformly bounded away from one.

In order to describe the structure of nearly uncoupled Markov chains that satisfy the two regularity conditions, we must introduce still more notation. We have observed that the vector v_y defined by (2.4) is a left eigenvector of B_y. Similarly the vector $u = (1, 1, \ldots, 1)^{\mathrm{T}}$ is a right eigenvector of B_y. By the remarks surrounding equation (2.5), we can find uniformly bounded matrices U and V of dimension $l \times (l-1)$ such that

$$(u\ U)^{-1} = (v_y\ V)^{\mathrm{T}}. \tag{2.9}$$

Because u and v_y are right and left eigenvectors of B_y,

$$(v_y\ V)^{\mathrm{T}} B_y (u\ U) = \begin{pmatrix} 1 & 0 \\ 0 & \tilde{A}_2 \end{pmatrix}; \tag{2.10}$$

that is the similarity transformation (2.10) block diagonalizes B_y, placing the eigenvalue one in the upper left and the remaining eigenvalues in the matrix $\tilde{A}_2$. Finally set

$$J = \begin{pmatrix} J_1 & 0 & \cdots & 0 \\ 0 & J_2 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & J_l \end{pmatrix}, \tag{2.11}$$

$$K = \begin{pmatrix} K_1 & 0 & \cdots & 0 \\ 0 & K_2 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & K_l \end{pmatrix}, \tag{2.12}$$

and

$$\tilde{A}_3 = K^{\mathrm{T}} A J. \tag{2.13}$$

We are now in a position to state the main result of this section, which asserts the existence and describes the structure of matrices $(x\ X_2\ X_3)$ and $(y\ Y_2\ Y_3)$ satisfying

$$(x\ X_2\ X_3)^{-1} = (y\ Y_2\ Y_3)^{\mathrm{T}} \tag{2.14}$$

and

$$(y\ Y_2\ Y_3)^{\mathrm{T}} A (x\ X_2\ X_3) = \mathrm{diag}(1, A_2, A_3). \tag{2.15}$$

Here A_2 is of order $l-1$ and A_3 is of order $n-l$. The proof may be found in [4].

Theorem 2.1. *Let A satisfy Regularity Conditions 1 and 2. Then for all sufficiently small ϵ the decomposition (2.14-2.15) exists. Moreover, there are matrices P and Q satisfying*

$$\|P\|, \|Q\| = O(\epsilon) \tag{2.16}$$

such that

$$\begin{array}{ll} 1.\ x = Su, & 2.\ y = T_y v_y, \\ 3.\ X_2 = SU + JP + O(\epsilon^2), & 4.\ Y_2 = T_y V + KQ, \\ 5.\ X_3 = J - SUQ^{\mathrm{T}} + O(\epsilon^2), & 6.\ Y_3 = K - T_y V P^{\mathrm{T}}, \\ 7.\ A_2 = \tilde{A}_2 + O(\epsilon^2), & 8.\ A_3 = \tilde{A}_3 + O(\epsilon^2). \end{array} \tag{2.17}$$

There are several comments to be made about this theorem. In the first place, it follows from (2.15) that

$$Y_i^{\mathrm{T}} A = A_i Y_i^{\mathrm{T}} \qquad (i = 1, 2). \tag{2.18}$$

This shows that the space spanned by the columns of Y_i is a left invariant subspace of A; that is, it is unchanged when it is transformed by A^{T}. The matrix A_i is the representation of A restricted to the column space of Y_i.

Since from (2.17) the powers of A satisfy

$$Y_i^{\mathrm{T}} A^s = A_i^s Y_i^{\mathrm{T}} \qquad (i = 1, 2), \tag{2.19}$$

the eigenvalues of A_i control the behavior of the Markov chain on the space spanned by Y_i. The asymptotic behavior of these eigenvalues is easily determined. From (1.7), (2.10) and (2.17) it is seen that

$$A_2 = I + O(\epsilon). \tag{2.20}$$

Consequently the eigenvalues of A_2 are near one, and as s becomes large A_2^s approaches zero slowly; that is, Y_2 corresponds to a slow transient of the Markov chain. On the other hand, from (2.6), (2.13) and (2.17) it is seen that

$$A_3 = \mathrm{diag}(C_1, C_2, \ldots, C_l) + O(\epsilon). \tag{2.21}$$

From Regularity Condition 2, the eigenvalues of the C_i are bounded away from one. Consequently, A_3^s approaches zero more swiftly than A_2^s; that is, Y_3 corresponds to a fast transient. This behavior of nearly uncoupled chains was first noted by Simon and Ando [5]. [We note in passing that a condition different from Regularity Condition 2 was used by the authors of this paper to establish the results in [4].

However, that condition is implied by Regularity Condition 2 along with (2.20) and (2.21).]

The spaces associated with the slow and fast transients are highly structured. For example, (2.17.4) shows that the space corresponding to the slow transient is essentially a subspace of space spanned by T_y; i.e., it is made up of pieces of the eigenvector y. This is why the Rayleigh–Ritz technique is so good at eliminating errors in the slow transient space; if the $\hat{z}_i$ are good approximations to the $\hat{y}_i$ [see (1.11)], then T_z contains a good approximation to the slow transient error and the Rayleigh–Ritz process uses it to purge the error.

On the other hand, the space associated with the fast transient is essentially spanned by K. This fact will be crucial in explaining why the Gauss–Seidel step tends to purge errors along the fast transient.

We turn now to the properties of the Rayleigh–Ritz step. The basic result requires yet another regularity condition, designed to keep the slow transient apart from the steady state. This can be done by keeping the eigenvalues of $\tilde{A}_2$ in (2.10) bounded away from one by a quantity proportional to ϵ. Rather than work directly with eigenvalues, we work with the norm of an appropriate matrix, as we did in Regularity Condition 2.

Regularity Condition 3. There is a constant M_3 such that

$$\|(I - \tilde{A}_2)^{-1}\| < M_3\epsilon^{-1} \tag{2.22}$$

With the third regularity condition added to the first two, the following theorem is valid [4].

Theorem 2.2. *Let A satisfy Regularity Conditions 1, 2, and 3. Let $z > 0$ be given with $\|z\|_1 = 1$. Let γ_i be defined by (1.17). Let $\tilde{z}$ be the vector produced by one step of the Rayleigh–Ritz step and let $\tilde{\gamma}_i$ be defined in analogy with (1.17). Then for all sufficiently small ϵ, γ_2 and γ_3 there are constants $N_2, N_3 > 0$ such that*

$$\tilde{\gamma}_i <= \epsilon N_2\gamma_2 + N_3\gamma_3 \qquad (i = 1, 2). \tag{2.23}$$

From this theorem it is seen that the Rayleigh–Ritz step is a γ_2 reducer. However, it is only effective when γ_3 is less than γ_2. Thus it must be used in conjunction with a γ_3 reducer. In the next section we shall show that the Gauss–Seidel step has this property.

3. Analysis of the Gauss–Seidel Step

In this section we shall be concerned with the analysis of the Gauss–Seidel step defined by (1.10). Although the details of the analysis are tedious, the underlying idea is straightforward. Let $z > 0$ have the expansion (1.16). Let $\tilde{z}$ be determined by (1.10) and write

$$\tilde{z} = \tilde{\gamma}_1 y + Y_2 \tilde{g}_2 + Y_3 \tilde{g}_3. \tag{3.1}$$

From (2.14) it follows that

$$\tilde{\gamma}_1 = \tilde{z}^{\mathrm{T}} x, \tag{3.2}$$

and

$$\tilde{g}_i^{\mathrm{T}} = \tilde{z}^{\mathrm{T}} X_i \qquad (i = 2, 3). \tag{3.3}$$

Thus the problem is to develop expressions for the products on the right hand sides of (3.2) and (3.3).

The first step is to express $\tilde{z}$ in matrix form. Referring to (1.2), let

$$A = D + L + U, \tag{3.4}$$

where L is strictly lower triangular and U is strictly upper triangular. After some manipulation, $\tilde{z}$ can be written in the form

$$\tilde{z}^{\mathrm{T}} = z^{\mathrm{T}} L[I - (I - D)^{-1} U]^{-1} (I - D)^{-1}. \tag{3.5}$$

If the expansion (1.16) for z is substituted into (3.5), the result is

$$\tilde{z}^{\mathrm{T}} = y^{\mathrm{T}} + g_2^{\mathrm{T}} Y_2^{\mathrm{T}} Z (I - D)^{-1} + g_3^{\mathrm{T}} Y_3^{\mathrm{T}} Z (I - D)^{-1}, \tag{3.6}$$

where

$$Z = L[I - (I - D)^{-1} U]^{-1} \tag{3.7}$$

(the simple form of the first term in the right-hand side of (3.6) is due to the fact that y is a fixed point of the Gauss–Seidel iteration).

The key to the analysis is to establish the behavior of the quantities in (3.6), which is done in the lemma below. The results may be summarized by saying that as ϵ approaches zero 1. $(I - D)^{-1}$ becomes large, but not too fast; 2. $(I - D)^{-1}$ remains bounded in the column space of X_3; 3. Z approaches zero as fast as $(I - D)^{-1}$ becomes large. Specifically,

Lemma 3.1. *Let A satisfy the three regularity conditions of Section 2. Then*

$$\begin{array}{l} 1.\ \|(I-D)^{-1}\| = O(\epsilon^{-1}) \\ 2.\ \|(I-D)^{-1}X_3\| = O(1) \\ 3.\ \|Z\| = O(\epsilon) \end{array} \tag{3.8}$$

Proof. From (1.3), to establish (3.8.1) it is sufficient to establish that $\|(I - A_{ii})^{-1}\| = O(\epsilon^{-1})$. In view of (2.6) and the uniform boundedness of the J_i and the K_i, it is sufficient to establish that

$$\begin{pmatrix} 1-\beta_i & -h_i^{\mathrm{T}} \\ -g_i & I - C_i \end{pmatrix} = O(\epsilon^{-1}). \tag{3.9}$$

Now

$$\begin{pmatrix} 1-\beta_i & -h_i^{\mathrm{T}} \\ -g_i & I - C_i \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -(1-\beta_i)^{-1}g_i & I \end{pmatrix} \begin{pmatrix} 1-\beta_i & -h_i^{\mathrm{T}} \\ 0 & I - C_i - (1-\beta_i)^{-1}g_i h_i^{\mathrm{T}} \end{pmatrix}, \tag{3.10}$$

which can be verified by multiplying the factors on the right hand side. In the appendix we shall show that

$$(1-\beta_i)^{-1} = O(\epsilon^{-1}). \tag{3.11}$$

Since $\|g_i\|$ and $\|h_i\|$ are of order ϵ, it follows from (3.10) and (3.11) that

$$\begin{pmatrix} 1-\beta_i & -h_i^{\mathrm{T}} \\ -g_i & I - C_i \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ O(1) & I \end{pmatrix} \begin{pmatrix} 1-\beta_i & O(\epsilon) \\ 0 & I - C_i + O(\epsilon) \end{pmatrix}, \tag{3.12}$$

From (2.7) and standard perturbation theory for matrix inverses [7, Ch. 4], $[I - C_i + O((\epsilon))]^{-1} = O(1)$. Hence from (3.12)

$$\begin{pmatrix} 1-\beta_i & -h_i^{\mathrm{T}} \\ -g_i & I - C_i \end{pmatrix}^{-1} = \begin{pmatrix} O(\epsilon^{-1}) & O(1) \\ O(1) & O(1) \end{pmatrix}, \tag{3.13}$$

which establishes (3.8.1).

To establish (3.8.2) note that by (2.17.5) it is sufficient to show that $(I - D)^{-1}J = O(1)$, or in view of the block diagonality of D and K that $(I - A_{ii})^{-1}J_i = O(1)$. From (2.6)

$$(I - A_{ii})^{-1}J_i = (x_i\ J_i) \begin{pmatrix} 1-\beta_i & -h_i^{\mathrm{T}} \\ -g_i & I - C_i \end{pmatrix}^{-1} (x_i\ J_i)^{-1}J_i. \tag{3.14}$$

Hence from (3.13)

$$(I - A_{ii})^{-1} J_i = (x_i \; J_i) \begin{pmatrix} O(\epsilon^{-1}) & O(1) \\ O(1) & O(1) \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = (x_i \; J_i) \cdot O(1), \tag{3.15}$$

and the result follows from the fact that $(x_i \; J_i)$ is uniformly bounded.

To establish (3.8.3) note that since $L = O(\epsilon)$ it is sufficient to show that

$$[I - (I - D)^{-1} U]^{-1} = O(1). \tag{3.16}$$

Set $\bar{U} = (I - D)^{-1} U$. Since $U = O(\epsilon)$, it follows from (3.8.1) that $\bar{U} = O(1)$. Since $\bar{U}$ is strictly lower triangular, the geometric series

$$(I - \bar{U})^{-1} = I + \bar{U} + \bar{U}^2 + \cdots \tag{3.17}$$

terminates. Thus $(I - \bar{U})^{-1} = O(1)$ which establishes (3.8.3) and the lemma.

With Lemma 3.1 established, the analysis of the Gauss–Seidel step amounts to little more than postmultiplying (3.6) by x, X_2 and X_3 and applying the lemma. For example,

$$\begin{aligned} \tilde{\gamma}_3 &= \|\tilde{z}^{\mathrm{T}} X_3\| \\ &= \|g_2\| \|Y_2^{\mathrm{T}} Z\| \|(I - D)^{-1} X_3\| + \|g_3\| \|Y_2^{\mathrm{T}} Z\| \|(I - D)^{-1} X_3\|. \end{aligned} \tag{3.18}$$

Hence from (3.8.2) and (3.8.3) it follows that there is a constant L^3 such that $\tilde{\gamma}_3 <= \epsilon L^3 (\gamma_2 + \gamma_3)$. The other bounds are obtained similarly.

Theorem 3.2. *In the notation introduced above, if A satisfies the three regularity conditions, then there are constants* L^i $(i = 1, 2, 3)$ *such that*

$$\begin{aligned} &a.\ |1 - \tilde{\gamma}_1| \le L^1 (\gamma_2 + \gamma_3), \\ &b.\ \tilde{\gamma}_2 \le L^2 (\gamma_2 + \gamma_3), \\ &c.\ \tilde{\gamma}_3 \le \epsilon L^3 (\gamma_2 + \gamma_3). \end{aligned} \tag{3.19}$$

Theorem 3.2 allows us to give a local convergence proof of the two step iteration. First assume that initially

$$L^1 (\gamma_2 + \gamma_3) \le \frac{1}{2}, \tag{3.20}$$

so that when the vector $\tilde{z}$ obtained from the Gauss–Seidel step is normalized to give a vector $\bar{z}$, the resulting $\bar{\gamma}_i$ satisfy

$$\begin{array}{l} b.\ \bar{\gamma}_2 \le 2L^2(\gamma_2+\gamma_3) \\ c.\ \bar{\gamma}_3 \le 2\epsilon L^3(\gamma_2+\gamma_3) \end{array} \tag{3.21}$$

In matrix notation (3.21) becomes

$$\begin{pmatrix} \bar{\gamma}_2 \\ \bar{\gamma}_3 \end{pmatrix} \le 2 \begin{pmatrix} L^2 & L^2 \\ \epsilon L^3 & \epsilon L^3 \end{pmatrix} \begin{pmatrix} \gamma_2 \\ \gamma_3 \end{pmatrix}. \tag{3.22}$$

If $\hat{z}$ denotes the result of applying a Rayleigh–Ritz refinement to $\bar{z}$, then from (2.23) it follows that

$$\begin{aligned} \begin{pmatrix} \bar{\gamma}_2 \\ \bar{\gamma}_3 \end{pmatrix} &\le 2 \begin{pmatrix} \epsilon N_2 & N_3 \\ \epsilon N_2 & N_3 \end{pmatrix} \begin{pmatrix} L^2 & L^2 \\ \epsilon L^3 & \epsilon L^3 \end{pmatrix} \begin{pmatrix} \gamma_2 \\ \gamma_3 \end{pmatrix} \\ &= 2\epsilon(N_2L^2+N^3L^3) \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \gamma_2 \\ \gamma_3 \end{pmatrix} \end{aligned} \tag{3.23}$$

It follows that

$$\hat{\gamma}_2+\hat{\gamma}_3 \le 4\epsilon(N_2L^2+N_3L^3)(\gamma_2+\gamma_3). \tag{3.24}$$

Thus if

$$4\epsilon(N_2L^2+N_3L^3) < 1, \tag{3.25}$$

then (3.20) remains satisfied, and the iteration converges. In other words the composite iteration consisting of alternating Gauss–Seidel and Rayleigh–Ritz steps converges provided ϵ is sufficiently small and the starting approximation is sufficiently good.

There are three comments to be made about these results. First, although we have applied Theorem 3.2 to analyze the case where a Rayleigh–Ritz step is alternated with a Gauss-Siedel step, in practice it may be preferable to perform two or more Gauss–Seidel steps. The best mix will depend on factors, such as the observed rates of convergence and the relative cost of each kind of step, which are best evaluated in the course of the iteration. We shall give some examples in the next section.

The second observation is that the analysis extends with little modification to the method of Takahashi [9]. His method differs from ours in the way intermediate quantities are scaled in the Gauss–Seidel step. Specifically, if we write

$$W_z = \mathrm{diag}(\|z_1\|_1 I_{n_1}, \ldots, \|z_l\|_1 I_{n_l}), \tag{3.26}$$

then the iterate $\tilde{z}$ produced by Takahashi's method satisfies

$$\tilde{z}^{\mathrm{T}} = z^{\mathrm{T}} L\Big(I - (I-D)^{-1} W_{\tilde{z}}^{-1} W_z U\Big)^{-1} (I-D)^{-1}. \tag{3.27}$$

It is easily shown that as $z \to y$, the matrix $W_{\tilde{z}}^{-1} W_z \to I$. Consequently, if ϵ is small enough and z is near enough y, the two methods generate almost identical iterates, both of which reduce the error by a factor uniformly less than one.

Finally we note that although the bounds derived above are sufficient to establish the convergence of the two-stage iteration, they by no means give an adequate description of how the iteration behaves in practice. For it turns out that the Gauss–Seidel step, in addition to being a γ_3 reducer, is also a γ_2 reducer. How this comes about is an open research problem.

4. Implementation and Examples

An important advantage of the two-stage iteration is that each of its steps is comparatively easy to implement. The Gauss–Seidel step (1.10) requires that the system of equations

$$\tilde{z}_j^{\mathrm{T}} (I - A_{jj}) = \Big(\sum_{i<j} \tilde{z}_i^{\mathrm{T}} E_{ij} + \sum_{i>j} z_i^{\mathrm{T}} E_{ij}\Big) \tag{4.1}$$

be solved for $j = 1, 2, \ldots, l$. The preferred method is to compute an LU factorization of the matrix $(I - A_j j)$ and use this factorization to solve the system [2]. Because the matrix does not change from iteration to iteration, the factorization need be done only once, which represents a great savings in computational effort. In fact, the floating-point operation count is approximately the cost of a single matrix-vector multiplication: n^2 flops,[1] less if advantage is taken of the sparsity of the matrix.

In the Rayleigh–Ritz step, the formation of B_z will require approximately the same amount of work as one Gauss–Seidel step. Since only the dominant left eigenvector of B_z is required and the corresponding eigenvalue is known, it should be computed by the inverse power method [7, Ch. 7]. This requires that an LU decomposition of $I - B_z$ be calculated at a cost of $l^3/3$ flops. In large problems this calculation will be insignificant compared to the computation of B_z, so

[1] A flop is one floating-point addition and one floating-point multiplication, usually accompanied by two array accesses.

that the Gauss–Seidel step and the Rayleigh–Ritz step will represent comparable computations.

To illustrate the procedure we consider two examples, based on a model investigated by Vantilborgh in [10], where further references may be found. The following is Vantliborgh's description of the model.

> A finite number N of active user terminals generates random requests for program execution. User programs are executed on a multiprogrammed basis by a CPU/Main Memory server S_1 and a paged secondary-memory server S_2. A program is admitted to the multiprogramming mix if less than M programs are jointly present at S_1 and S_2; programs not admitted to this mix are kept waiting in a queue Q_3. At the end of a service, a program generates a disk request with probability δ, requires another quantum of execution with probability ϕ, or terminates. We use i_1 and i_2 to denote the congestion at S_1 and S_2.
>
> We assume
>
> (i) The think time of a user has a negative exponential distribution with parameter λ; [Throughout our examples we choose $\lambda = 0.001$.]
>
> (ii) S_1 and S_2 have exponentially distributed service times with parameters $\mu_1(i_1)$ and $\mu_2(i_2)$; [As in Vantilborgh, we choose the specific values $\mu_1(i_1) = 64/(i_1 + 16)$ and $\mu_2(i_2) = 3i_2/(i_2 + 6)$.]
>
> (iii) ϕ, and δ are independent of the state of the network; [We choose $\phi = 0.03$ and $\delta = 0.95$.]

In our first experiment with this model, we choose values of $N(6)$ and $M(3)$ so that the resulting probability matrix is small enough (order 22) to analyze completely using the QR algorithm [6]. This permits us to compute the norms γ_1 and γ_2 of the errors along the slow and fast transient subspaces. Table 4.1 presents the results first of alternating Rayleigh–Ritz steps with Gauss–Seidel steps and then of following a Rayleigh–Ritz step with five Gauss–Seidel steps. In both cases the starting vector was the vector of all ones. In the column labeled "step", the I indicates the initial values of γ_2 and γ_3, RR indicates the values after a Rayleigh–Ritz step, and GS the values after a Gauss–Seidel step. It is seen from this table, that increasing the number of Gauss–Seidel steps does not improve the convergence (experiments not summarized in the table show that an intermediate number of Gauss–Seidel steps does not help either).

The results also show that the Gauss–Seidel step reduces γ_2, although not as dramatically as a well-timed Rayleigh–Ritz step. This phenomena, which was al-

Vantilborgh Model $N = 6$ $M = 3$					
step	γ_2	γ_3	step	γ_2	γ_3
I	4.2E+00	7.2E+00	I	4.2E+00	7.2E+00
RR	5.8E−03	5.5E−03	RR	5.8E−03	5.5E−03
GS	2.5E−03	6.5E−05	GS	2.5E−03	6.5E−05
RR	3.9E−05	3.6E−04	GS	4.9E−04	1.4E−07
GS	1.6E−05	2.5E−07	GS	1.3E−04	3.3E−08
RR	2.9E−07	2.6E−06	GS	3.6E−05	9.7E−09
GS	1.2E−07	1.6E−09	GS	1.1E−05	2.9E−09
RR	2.1E−09	1.9E−08	RR	1.5E−07	1.4E−06
GS	8.4E−10	1.1E−11	GS	6.1E−08	9.3E−10
RR	1.5E−11	1.3E−10	GS	1.8E−08	3.3E−12
GS	6.0E−12	7.6E−14	GS	4.5E−09	1.1E−12
RR	1.3E−13	9.4E−13	GS	1.2E−08	3.2E−13
GS	8.8E−14	8.0E−16	GS	3.5E−10	9.5E−14
			RR	5.6E−12	5.0E−11
			GS	2.2E−12	3.4E−14
			GS	6.6E−13	3.0E−16
			GS	1.9E−13	3.0E−16
			GS	9.0E−14	3.0E−16
			GS	6.6E−14	3.0E−16

Table 4.1:

luded to in the last section, represents a gap in our understanding of the composite algorithm.

For the second example we choose $N = 50$ and $M = 30$, which gives a matrix of order 1,116 with diagonal blocks of order $1, 2, 3, \ldots, 29, 30, 31, 31, \ldots, 31$. The remaining parameters were left unaltered. Since the matrix is too large to analyze into invariant subspaces, we cannot compute γ_2 and γ_3. Instead we compute the error in the steady-state vector, which was obtained by iterating the two-stage iteration to convergence.

Table 4.2 shows the number of iterations required to achieve a given accuracy for a Rayleigh–Ritz step followed by a fixed number of Gauss–Seidel steps. It is seen that the best behavior is achieved when each Rayleigh–Ritz step is followed by three Gauss–Seidel steps.

Vantilborgh Model $N = 50$ $M = 30$ No. of Steps to Attain A Given Accuracy					
Decimal	Number of G–S Steps				
Places	1	2	3	4	5
2	5	4	5	6	7
3	7				
4	9	7	9	11	13
5	12	10			
6	16	13	13	16	19
7	20	16			
8	25	19	17	21	25
9	30	23	21		
10	36	27	25	26	31
11	42	31	29	31	
12	52	38	33	36	37
13	60	44	38	38	43

Table 4.2:

Appendix: Proof of Equation (3.11)

Let

$$X = \begin{pmatrix} 0 & 0 \\ 0 & I - \tilde{A}_2 \end{pmatrix}, \tag{A.1}$$

where A_2 is defined by (2.10). We observe that there cannot be two vectors w_1 and w_2 of norm one that remain orthogonal as $\epsilon \to 0$ and satisfy $w_i^{\mathrm{T}} X = o(\epsilon)$. For otherwise, there would be a linear combination $w_3 = (0\ \bar{w}_3^{\mathrm{T}})^{\mathrm{T}}$ of w_1 and w_2 that satisfies $\|w_3\| = 1$ and $w_3^{\mathrm{T}} X = o(\epsilon)$. It then follows that $\bar{w}_3^{\mathrm{T}}(I - \tilde{A}_2) = o(\epsilon)$, contradicting Regularity Condition 3. Since $I - B_y$ is similar to X and the similarity transformation is uniformly bounded, $I - B_y$ likewise cannot have two approximate null vectors that map into quantities of $o(\epsilon)$. We shall establish (3.11) by showing that if $1 - \beta_1 = o(\epsilon)$ then the matrix $I - B_y$ indeed has two such approximate null vectors.

The matrix $I - B_y$ has the form

$$I - B_y = \begin{pmatrix} 1 - \beta_1 & -h^{\mathrm{T}} \\ -g & I - B_2 \end{pmatrix}. \tag{A.2}$$

Since $(I - B_y)u = 0$, where u is the vector consisting of all ones, if $1 - \beta_1 = o(\epsilon)$ then we must also have $\|h\| = o(\epsilon)$. Thus $w_1 = (1\ 0)^{\mathrm{T}}$ is one $o(\epsilon)$ approximate null vector.

We claim that there is a vector $\bar{w}_2$ with $\|\bar{w}_2\| = 1$ such that $\bar{w}_2^{\mathrm{T}}(I - B_2) = o(\epsilon)$. For otherwise, the perturbation theory in [7, p. 295] would apply to show that there is a left eigenvector of $I - B_y$ of the form $(1\ o(1)$ corresponding to an eigenvalue that is $o(\epsilon)$ in size. Since, by Regularity Condition 3, there is only one such eigenvalue, namely the zero eigenvalue, the eigenvector must be a multiple of v_y. But by Regularity Condition 1 the components of v_y cannot approach zero — a contradiction.

Since $(-g\ I - B_2)u = 0$ it follows that $\bar{w}_2^{\mathrm{T}} g = o(\epsilon)$. Thus $w_2 = (0\ \bar{w}_2^{\mathrm{T}})^{\mathrm{T}}$ is a second $o(\epsilon)$ approximate null vector of $I - B_y$. Since w_1 and w_2 are orthogonal, we have arrived at a contradiction, and equation (3.11) is established.

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